# ENERGY INNOVATION HUBS

## Energy Innovation Hub for Extreme Materials

A new activity introduced in FY 2010, the Extreme Materials Innovation Hub supports research into advanced materials for nuclear technologies, such as reactors, waste storage and disposal technologies, components, fuels, cladding and waste forms. Recent experiments and experience indicate that dramatically improved materials for use in various applications that face extreme environments including high-radiation and high-temperature are possible. To achieve these transformational advances in materials performance a science-based approach is needed. The science-based approach combines fundamental understanding of materials behavior at micro-structural level combined with phase-field and atomistic theories, advanced experimental and characterization techniques to guide the development of data-bases at the micro-structural level and lower length-scales, and advanced modeling and simulation tools.

The Extreme Materials Innovation Hub will be a competitively awarded. This Hub will focus and integrate the national effort to develop and test advanced materials needed to transform the performance of nuclear energy systems. Advanced materials have the potential to dramatically improve reactor performance, fuel cycle economics and the behavior of waste forms. The use of advanced materials for component replacement in the existing light water reactor fleet may improve safety margins and reduce the frequency of component replacements. For advanced reactors, development of better materials could improve efficiency of electricity generation as well as improved waste management strategies. Furthermore, fundamental understanding of materials and being able to tailor materials design to specific performance requirements will reduce the uncertainties associated with waste form performance in various environments.

The Extreme Materials Innovation Hub complements the Integrated Performance and Safety Codes effort of the Modeling and Simulation Hub. It will also make extensive use of the capabilities developed by the Office of Science through its Advanced Computing program. It will require, however, a different approach and the development of different tools.

## Energy Innovation Hub for Modeling and Simulation

The design and licensing of the current fleet of reactors was based on conventional engineering processes that relied on a series of evolutionary steps that moved from prototypes to demonstrations to commercial power plants. Without significant experimentation, validation, and verification, the engineering development processes for the current fleet of reactors had to ensure that the designs were sufficiently conservative to cover the lack of precise models to simulate system behaviors under steady-state and transient conditions.

The newest generation of plant designs (Generation III+) makes use of improved methods where available, but there has been no systematic industry-wide effort to upgrade mechanistic models to reflect a fundamental understanding of the underlying physical phenomena. The result is that the designs still rely on substantial conservative engineering judgment. This is both understandable and appropriate because the new designs, although incorporating many advances, are not fundamentally different from the well-understood plants now operating.

The Modeling and Simulation Hub will focus on providing validated advanced modeling and simulation tools necessary to enable fundamental change in how the U.S. designs and licenses nuclear power and waste management technologies. This has the potential to improve the performance and reduce the costs of new nuclear facilities.

The Modeling and Simulation Hub will be competitively awarded. This Hub will work to accelerate the predictive modeling and simulation capability that could be used in many technology areas.

## Solar Electricity Energy Innovation Hub

The Solar Electricity Hub will incorporate cutting edge research that may include both PV and CSP technology areas. PV research will be the primary focus of the hub with emphasis on the synthesis and modeling of disruptive PV device structures and processes to enable conceptual and cost breakthroughs. More specifically, projects will incorporate optical, electrical, and thermal phenomena, previously demonstrated only at the material level, into a PV device structure in order to demonstrate the technical viability and economic promise of the approach. Additionally, radical processes which promise disruptive 5 to 10x reductions in feedstock, processing costs or capital expenditure will be explored at the laboratory scale. The CSP portion would likely focus on materials research related to reflector coatings (e.g. glass, aluminum, polymers), thermal receivers, and high temperature heat transfer fluids and thermal storage media. The grants will not provide "bricks and mortar," but up to $10 million of the $35 million award may be used for retrofits and capital equipment.

## Energy Innovation Hub for Carbon Capture and Storage

In FY 2010, the Energy Innovation Hub for Carbon Capture and Storage will focus on enabling fundamental advances and discovery of novel and revolutionary capture/separation approaches to dramatically reduce the energy penalty and costs associated with CO2 capture. Both computational and experimental studies will be carried out for surface interactions of CO2 and other gases, novel solvents/sorbents, and chemical, physical, and biological separation approaches. There are a number of technical issues associated with Carbon Capture and Storage (CCS), the most challenging of which is to significantly reduce the high cost of capturing CO2 from large stationary emission sources such as coal power plants and transporting for permanent sequestration in either a liquid or solid form. Cost reductions are an imperative for CCS to be a viable technology option in the U.S, and in large coal-dependent developing nations.

## Focus of Grid Materials, Devices and Systems Hub

The grand challenges for the Grid Materials, Devices and Systems Hub activity include:

- Development of advanced Power Electronics materials, devices and integrated systems for cost-effective, high- voltage energy conversion and flow control;
- Discovery and design of "smart" material-based sensors and devices for long distance energy transfer; fault mitigation, including condition monitoring and fault diagnostics; and system configuration.

In FY 2010, an Innovation Hub will be solicited through a competitive process. The hub will involve national laboratories, universities, material producers, device and equipment manufacturers, and other public and private sector stakeholders. It will focus on *power electronics materials that leverage* recent advances by DARPA in wide bandgap semiconductors, including Silicon Carbide (SiC) and Gallium Nitride (GaN). Major challenges facing these technologies will be addressed, including materials deficiencies that contribute to fundamental limitations of the device technology, and cost and performance issues that are directly related to materials and the control of materials processes. Also, in FY 2010, research focusing on *smart material-based sensors and devices will be established.* The Hub will initiate efforts in embedded sensor applications for "smart" materials. These applications will lead to the development of self-diagnostics of operating conditions of various devices. Integrating this self- diagnostics capability with algorithms for asset managers through broader "smart grid" communications will help manage the growing need to replace and upgrade existing infrastructure, and to reduce catastrophic failures, maintenance costs, and improve the overall reliability of the power system.

## Energy Innovation Hub – Fuels from Sunlight

Basic research has provided enormous advances in our understanding of the subtle and complex photochemistry associated with the natural photosynthetic system. Similar advances have been made in purely inorganic photo-catalytic approaches to split water or photoreduce carbon dioxide. Yet, we still lack sufficient knowledge of the natural process and adequate control of artificial systems to design solar fuel generation processes with the efficiency, sustainability, or economic viability required. A Hub focused on making fuels from sunlight would aim at developing a direct solar fuel conversion system with overall conversion efficiency that produces fuels with sufficient energy content to enable the transition to proof-of-concept prototyping. The scale of the scientific challenge associated with this goal is daunting, but not insurmountable, and will require drawing expertise and premier scientific talent from the disciplines of chemistry, physics, materials sciences, biology, and engineering.

In FY 2010, research will be included in the following areas. Potential approaches to the challenge of producing fuels from sunlight that the Hub might adopt include the following:

- Replicating or reverse engineering the natural photosynthetic system with inorganic materials or hybrid bio-inorganic systems. Advances here require a more profound understanding of the subtle and complex chemistry of plant life, particularly in understanding the marvelous ability by which plants regulate the photosynthetic apparatus and repair themselves when damaged, both critical factors in the construction of a robust, man-made solar fuel generator.
- Using solar photovoltaics to drive the splitting of water or the reduction of carbon dioxide in an electrochemical cell, which requires the design and discovery of novel nano-engineered materials that catalyze the water splitting reaction and that are efficient, cost effective, environmentally benign, and have long-term stability and reliability.
- Artificially connecting biochemical systems that can combine water, sunlight, and even carbon dioxide to produce hydrogen or another chemical fuel in a man-made chemical reactor. The key to this approach is identifying the "software" for the synthetic cell, which can guide the process to the desired product.

## Energy Innovation Hub – Batteries and Energy Storage

Recent developments in nanoscience and nanotechnology offer tantalizing clues on promising scientific directions that may enable conceptual breakthroughs. They include the abilities to synthesize novel nanoscale materials with architectures tailored for specific electrochemical performance, to characterize materials and dynamic chemical processes at the atomic and molecular level, and to simulate and predict structural and functional relationships using modern computational tools.

Based on this, radically new concepts in materials design can be developed for producing storage devices with materials that are abundant and low in manufacturing cost, are capable of storing higher energy densities, have long cycle lifetimes, and have high safety and abuse tolerance. Together, these new capabilities provide the potential for addressing the gaps in cost and performance separating the current electrical energy storage technologies and those required for sustainable utility and transportation needs. In FY 2010, research will be included in the following areas. Fundamental performance limitations of energy storage systems are rooted in the constituent materials making up an electrical energy storage device, and novel approaches are needed to develop multifunctional electrical energy storage materials that offer new self-healing, self-regulating, failure-tolerant, impurity-sequestering, and sustainable characteristics. The Hub would address a number of specific areas of research for both batteries and electrochemical capacitors that have been identified in the BES workshop report *Basic Research Needs for Electrical Energy Storage. These include:*

- Efficacy of structure in energy storage—new approaches combining theory and synthesis for the design and optimization of materials architectures including self-healing, self-regulation, failure tolerance, and impurity sequestration.
- Charge transfer and transport—molecular scale understanding of interfacial electron transfer. Electrolytes—electrolytes with strong ionic solvation, yet weak ion-ion interactions, high fluidity, and controlled reactivity.
- Probes of energy storage chemistry and physics at all time and length scales—analytical tools capable of monitoring changes in structure and composition at interfaces and in bulk phases with spatial resolution from atomic to mesoscopic levels and temporal resolution down to femtoseconds.
- Multi-scale modeling—computational tools with improved integration of length and time scales to understand the complex physical and chemical processes that occur in electrical energy storage processes from the molecular to system scales.

## Energy Innovation Hub: Energy Efficient Building Systems Design

DOE proposes to establish multi-disciplinary Energy Innovation Hubs (Hubs) to address the basic science, technology, economic, and policy issues hindering the ability to become energy secure and economically strong while being good stewards of the planet by reducing GHG emissions. The main focus of the hub is to push the current state-of-the-art energy science and technology toward fundamental limits and support high-risk, high- reward research projects that produce revolutionary changes in how the U.S. produces and uses energy. The hubs are inspired by the Bell Labs research model, which produced the transistor, the building block of modern computers. Their objective is to focus a high-quality team of researchers on a specific question and to encourage risk taking that can produce real breakthroughs, as opposed to the typical, more cautious approach that can result in meaningful, but often only incremental, improvements to existing technology. DOE will encourage risk-taking by making the initial grant period five years, renewed thereafter for up to 10 years. Any funding after 10 years would be predicated on "raising the bar" above that needed for simple renewal. The grants will not provide "bricks and mortar," but up to $10 million of the $35 million award may be used for capital equipment. In FY 2010, BT will establish an R&D Hub that focuses on energy efficient building systems design. This hub will work on integrating smart materials, designs, and systems to tune building usage to better conserve energy, as well as maximizing the functioning of lighting, heating, air conditioning, and electricity to reduce energy demand. Areas of interest include improved exterior shell materials, membranes of energy efficient windows, insulation, improved approaches to building design, systems control, and energy distribution networks.